



High-resolution spectroscopy of gases at elevated temperatures for industrial applications

Fateev, Alexander; Clausen, Sønnik

Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Fateev, A. (Author), & Clausen, S. (Author). (2012). High-resolution spectroscopy of gases at elevated temperatures for industrial applications. Sound/Visual production (digital)

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

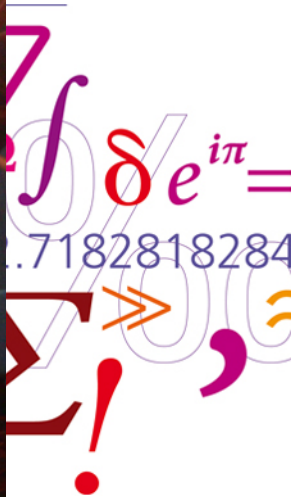
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

High-resolution spectroscopy of gases at elevated temperatures for industrial applications

Alexander Fateev and Sønnik Clausen

Optical Diagnostics Group,

DTU Chemical Engineering, Frederiksborgvej 399, Roskilde, DK-4000, Denmark

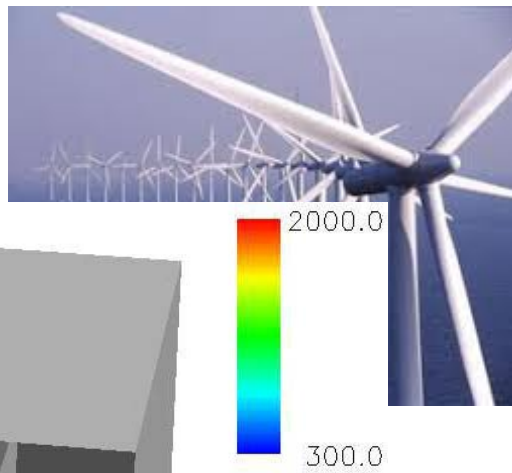


DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

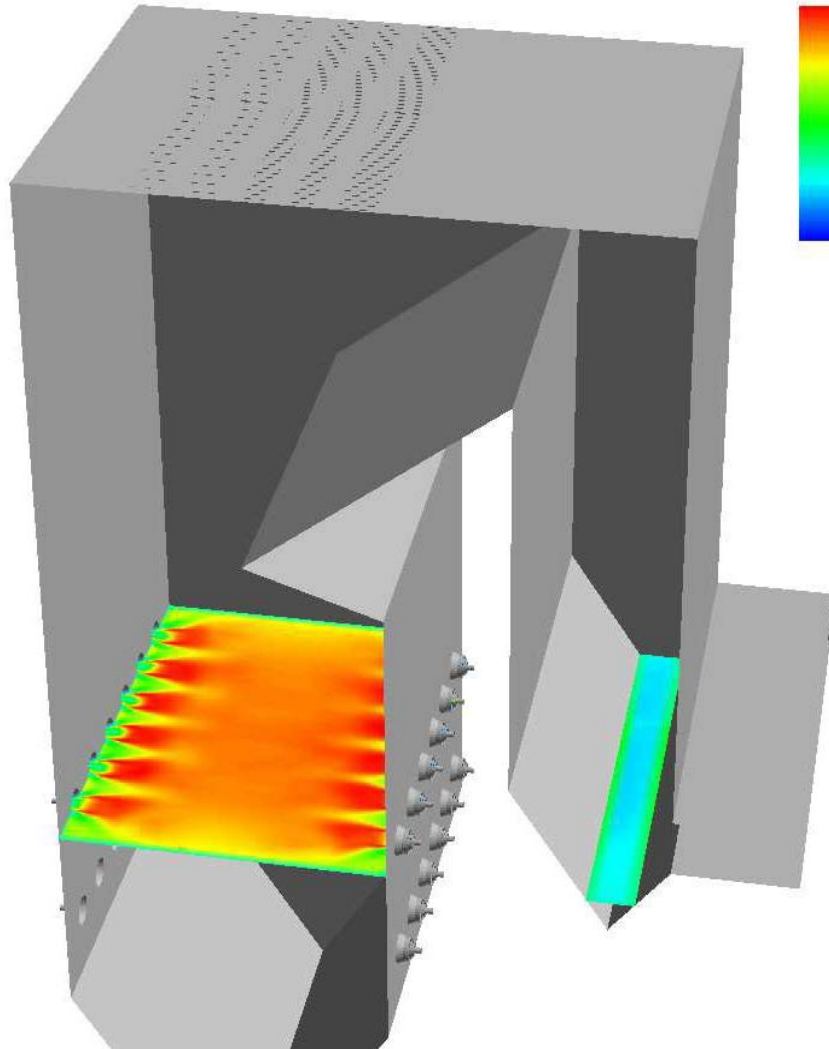
Outline

- Large scale measurements: why?
- Basic research: how it's made
- High resolution spectroscopy in flow gas cells: H₂O and CO₂
- SO₃ project: the story
- Conclusions

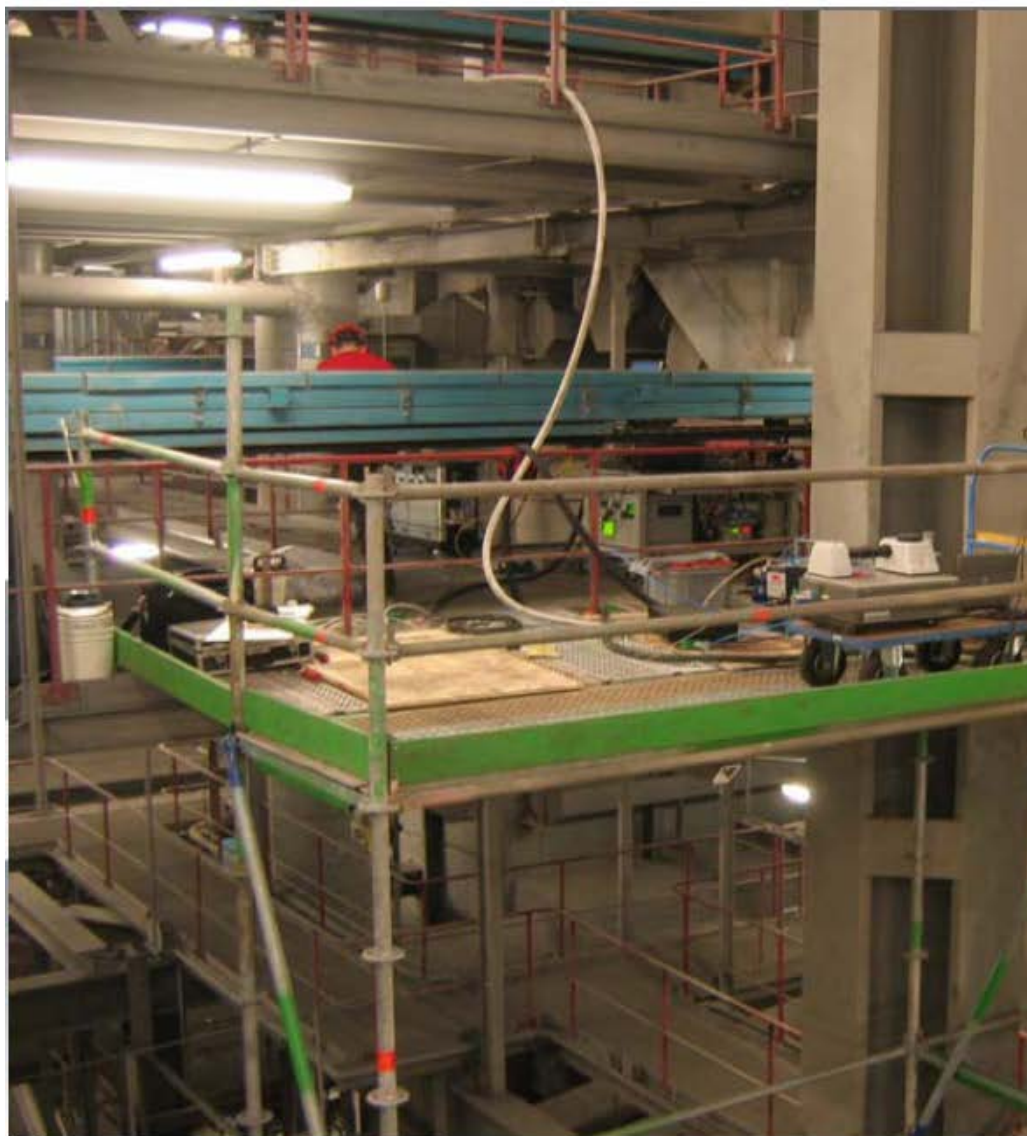
Green Energy...



... well



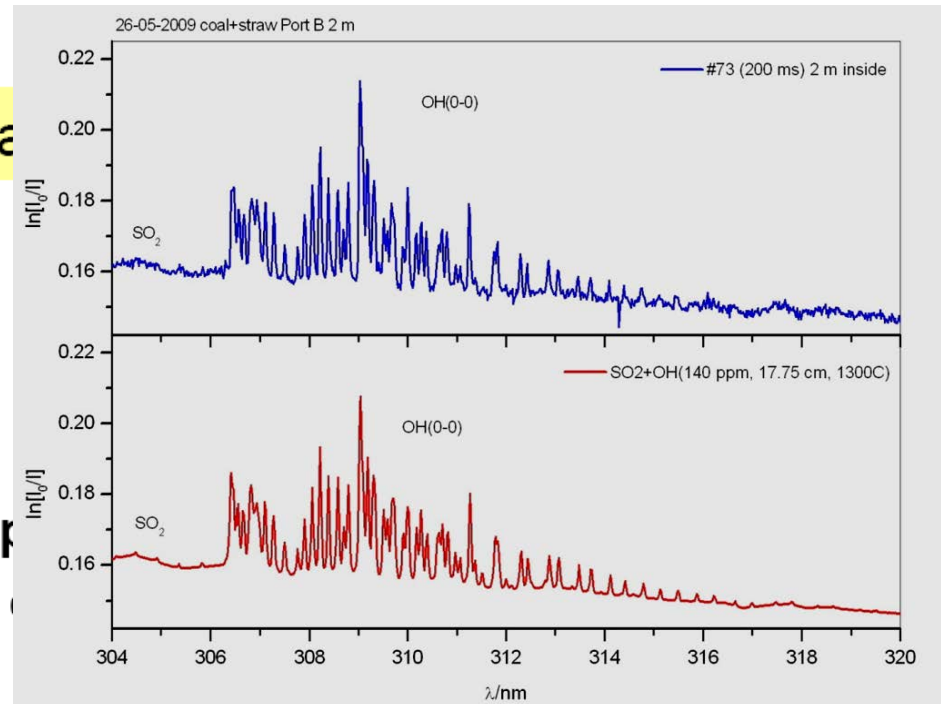
Large scale measurements



Large scale measurements

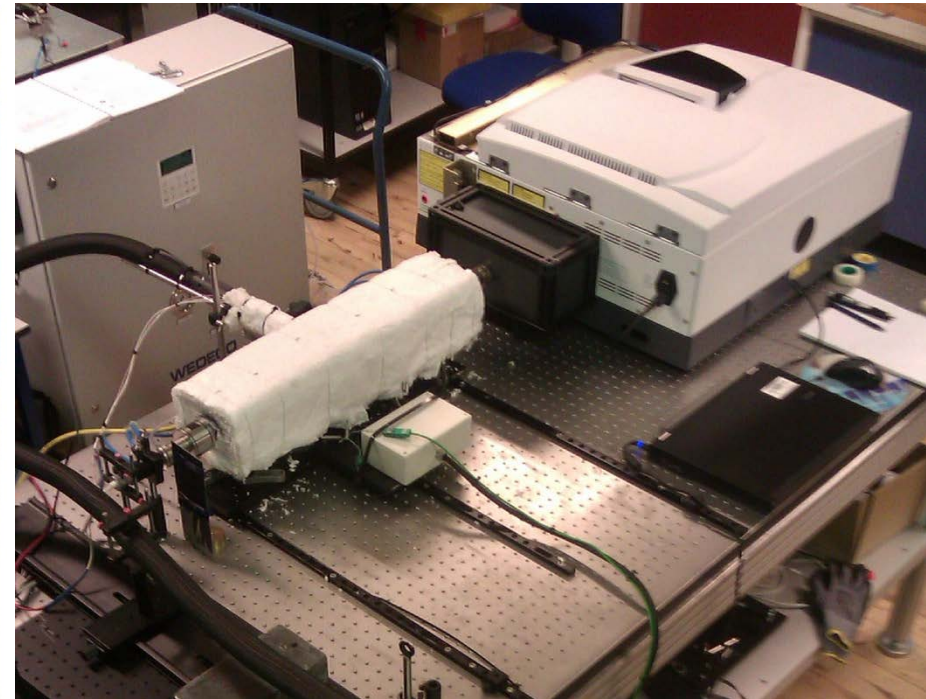
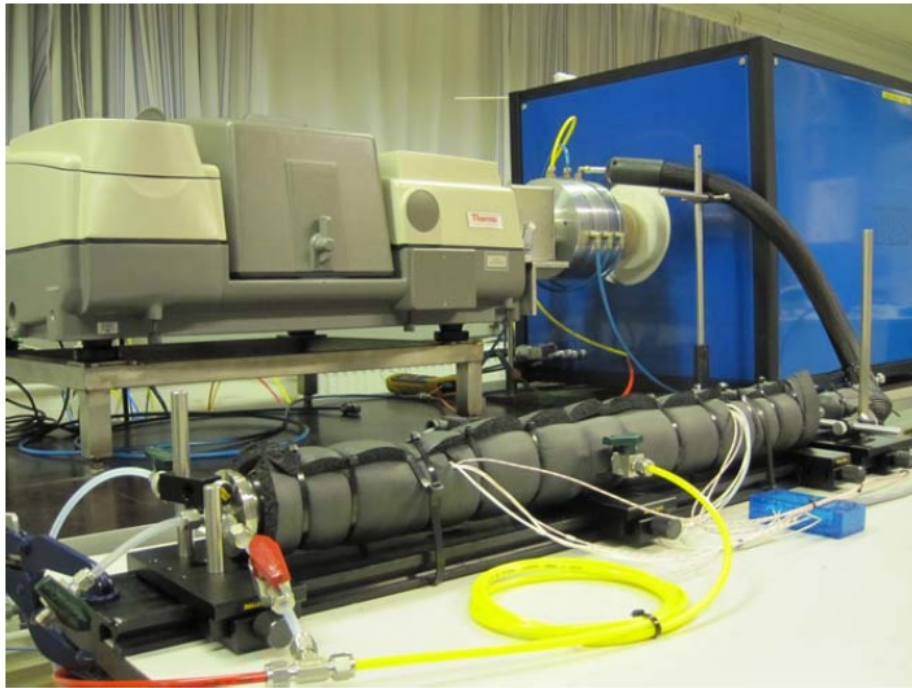
Fiber optical probes

- FTIR spectroscopy (emission): >5 m, 45 mm probe
 H_2O , CO_2 , CO , C_xH_y , HCl , etc. + T_{gas} + T_{par} + ϵ
- UV spectroscopy (transmission): 9 m, 60 mm probe
 SO_2 , NO , O_2 , etc.



Basic research

- focus on optical properties (TRS, ABS) of gases at temperatures up to 1600C;
- validation/building databases (e.g. HITRAN/HITEMP/CDSD...);
- high-resolution spectroscopy ($0.125\text{ cm}^{-1}/0.016\text{ nm}$) of “major” and “minor” (or trace) gases : [CO₂](#), [H₂O](#), [SO₂](#), [NH₃](#), [SO₃](#), [H₂S](#), [OCS](#), [HCL](#), [CH₃Cl](#), [PAH's](#) etc;
- various hot gas cells with highly-uniform temperature profiles ($\pm 0.5\text{C}$).

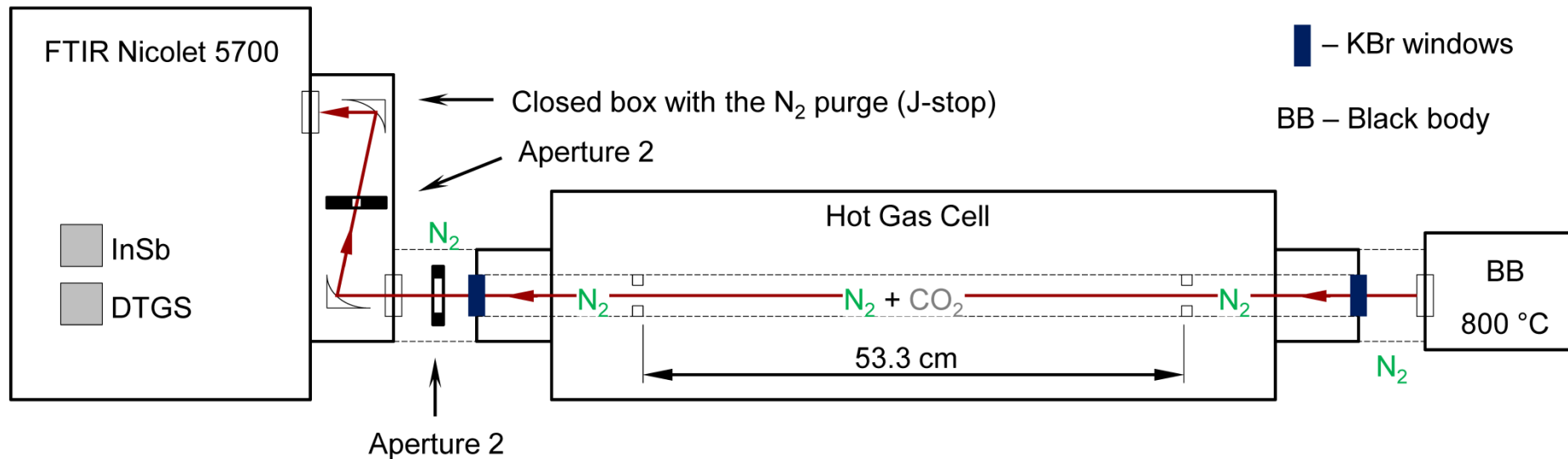


DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

Experimental set up

Includes:

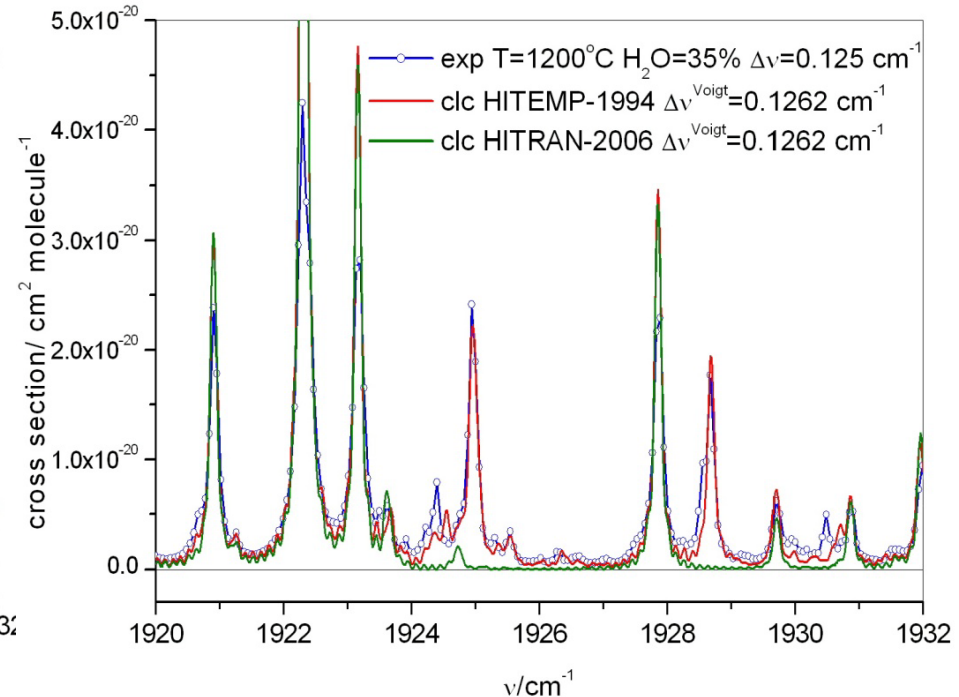
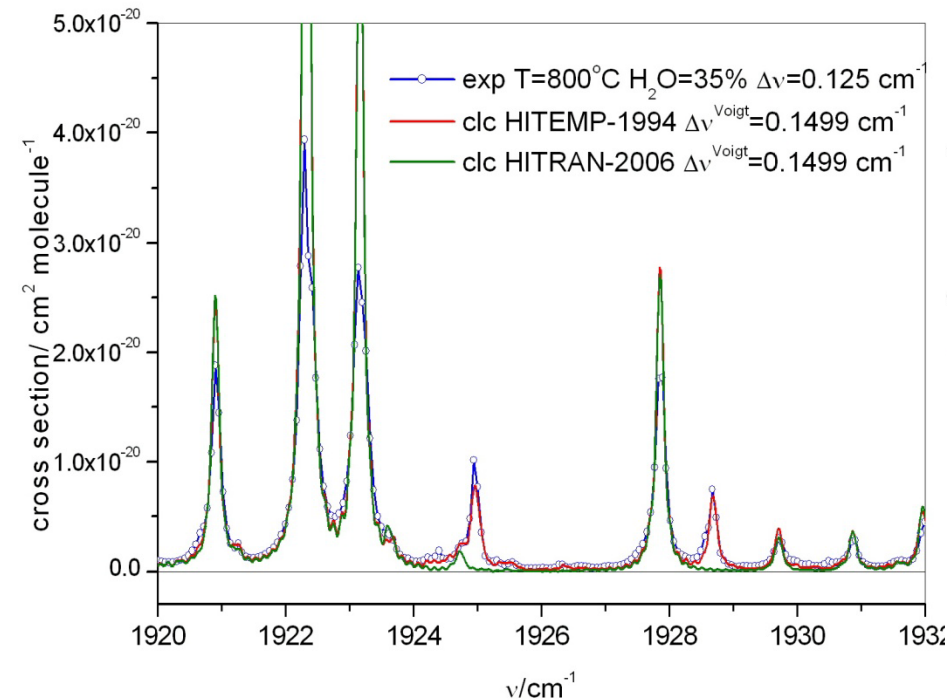
- a gas cell;
- a high-resolution FTIR spectrometer (Nicolet or Agilent);
- a light source (BB).



Examples: H₂O absorption cross sections

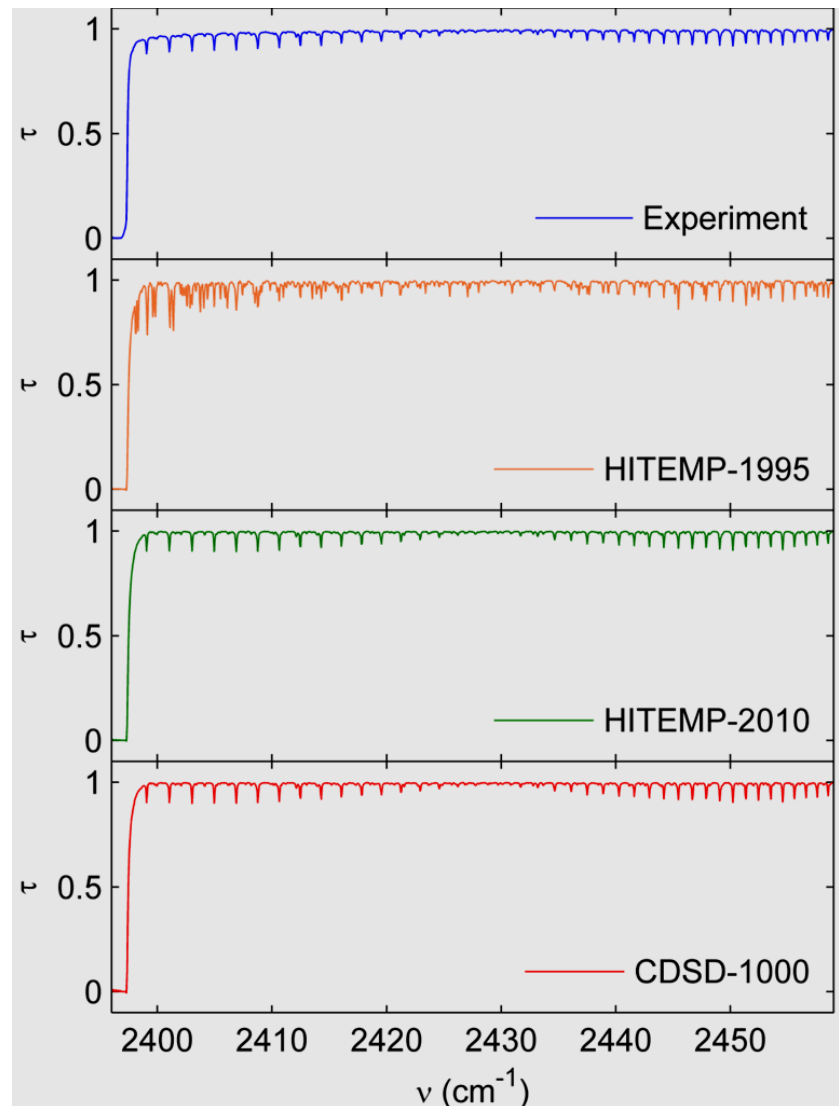
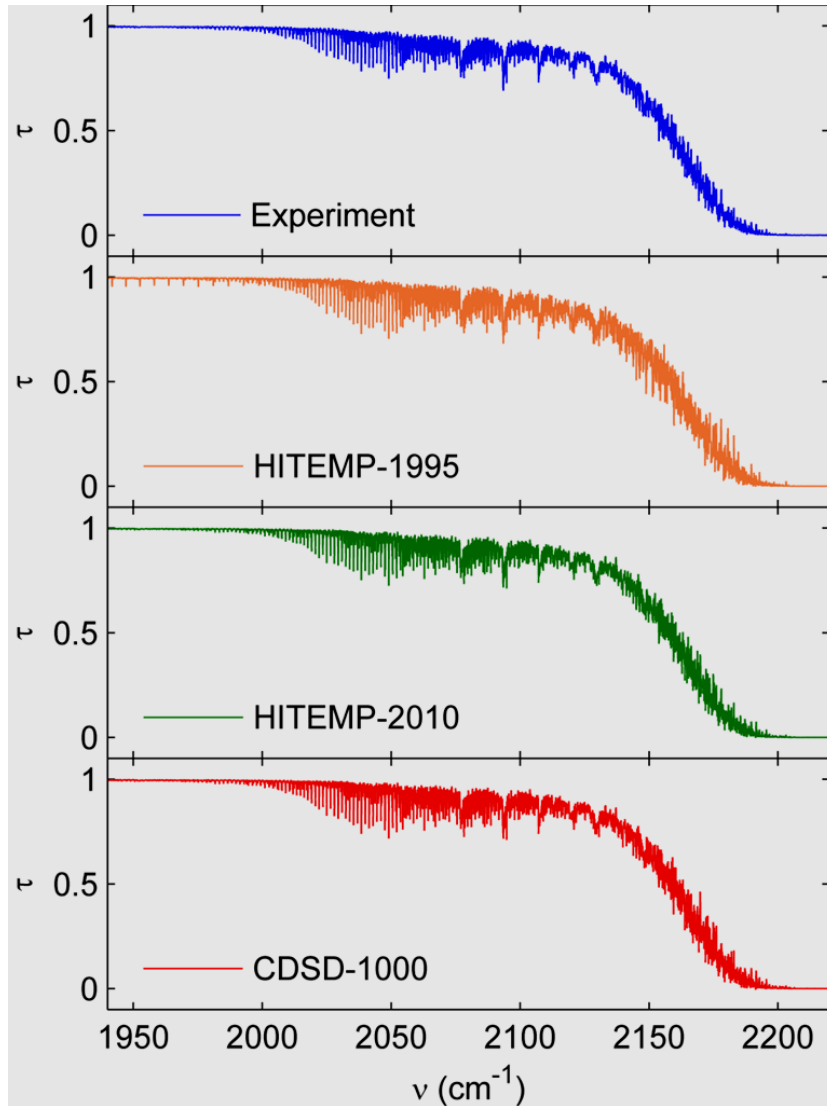
T=800C

T=1200C

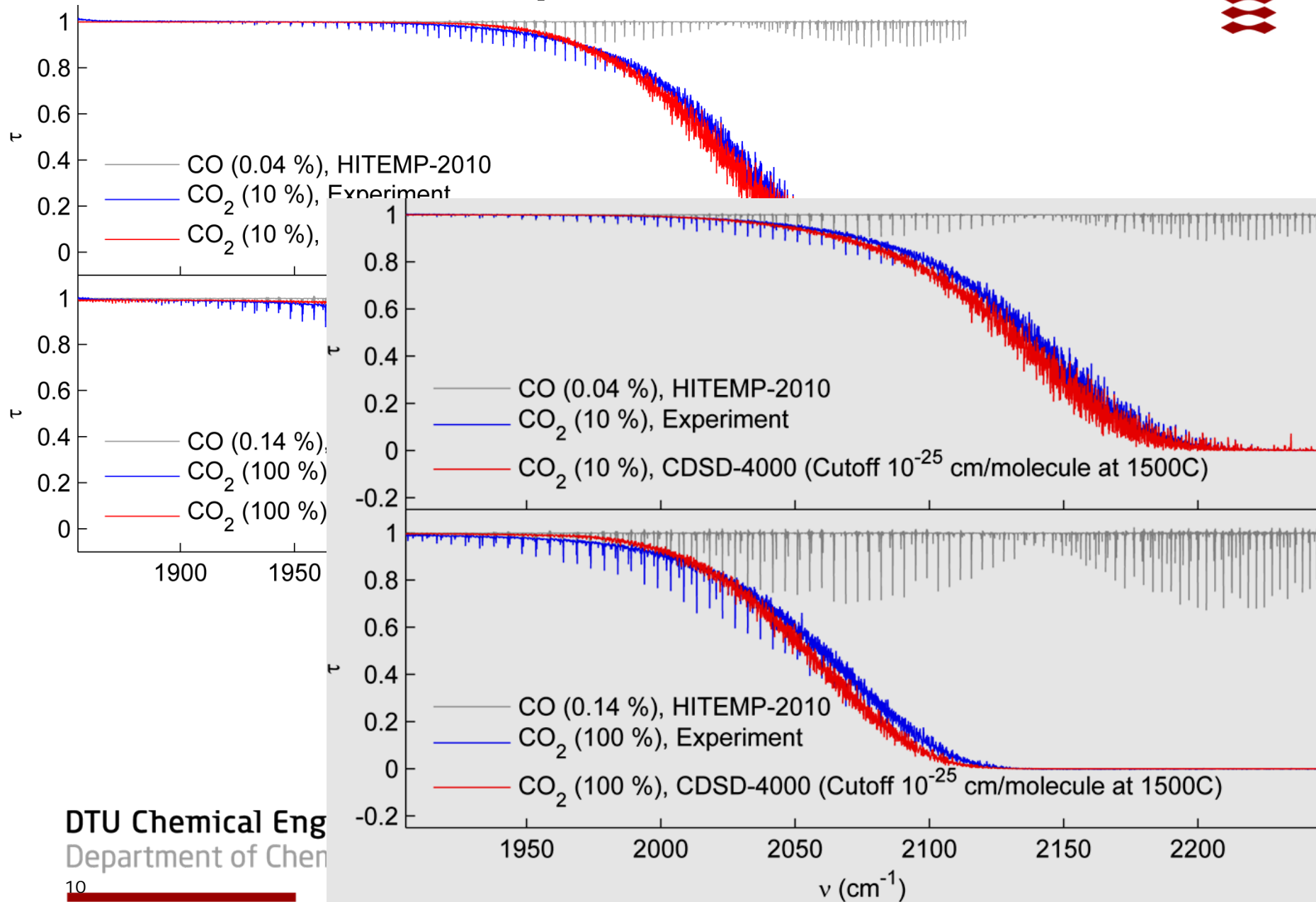


- Good agreement between EXP and CLC(HITEMP-1994);
- Different FWHM values of the H₂O single lines for H₂O(35%) in N₂ and H₂O(35%) in CO₂ (oxyfuel combustion).

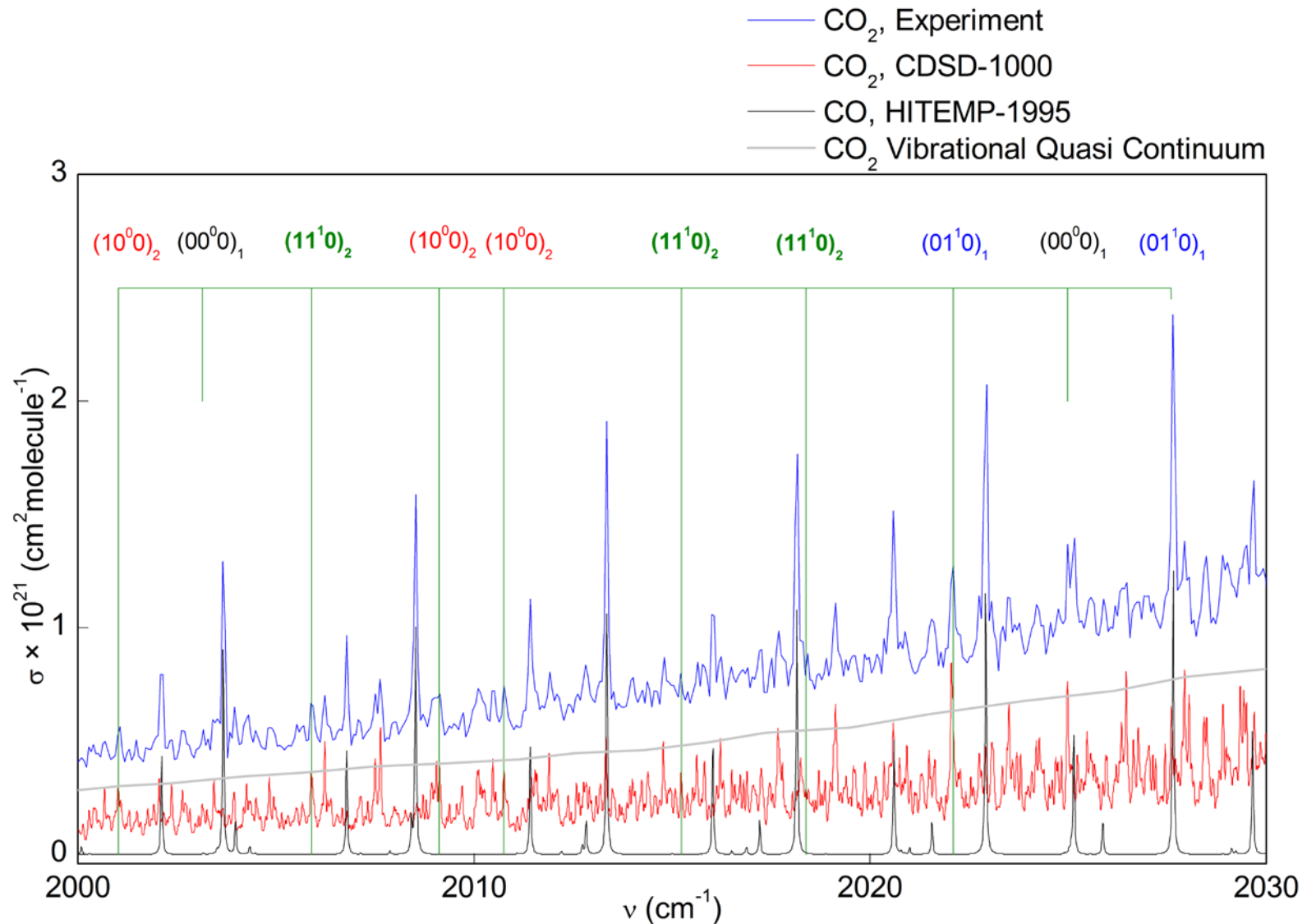
CO2 transmission spectra: 727C



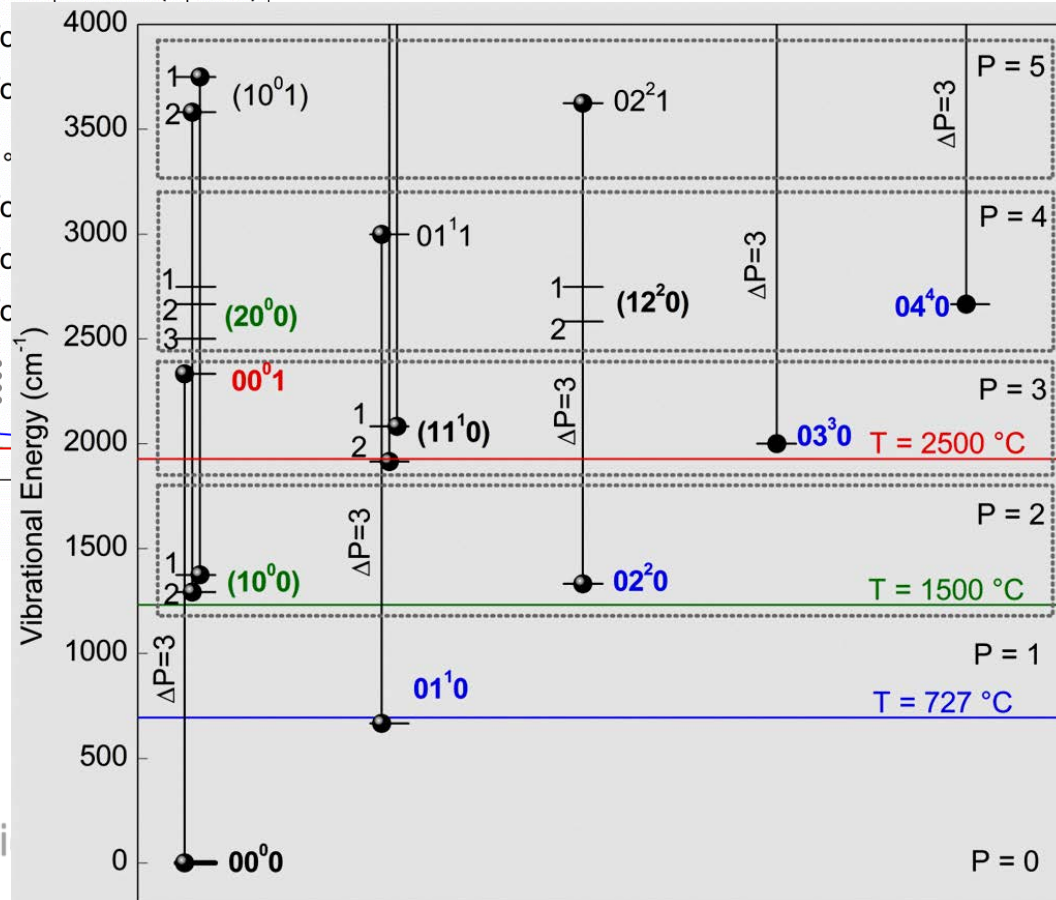
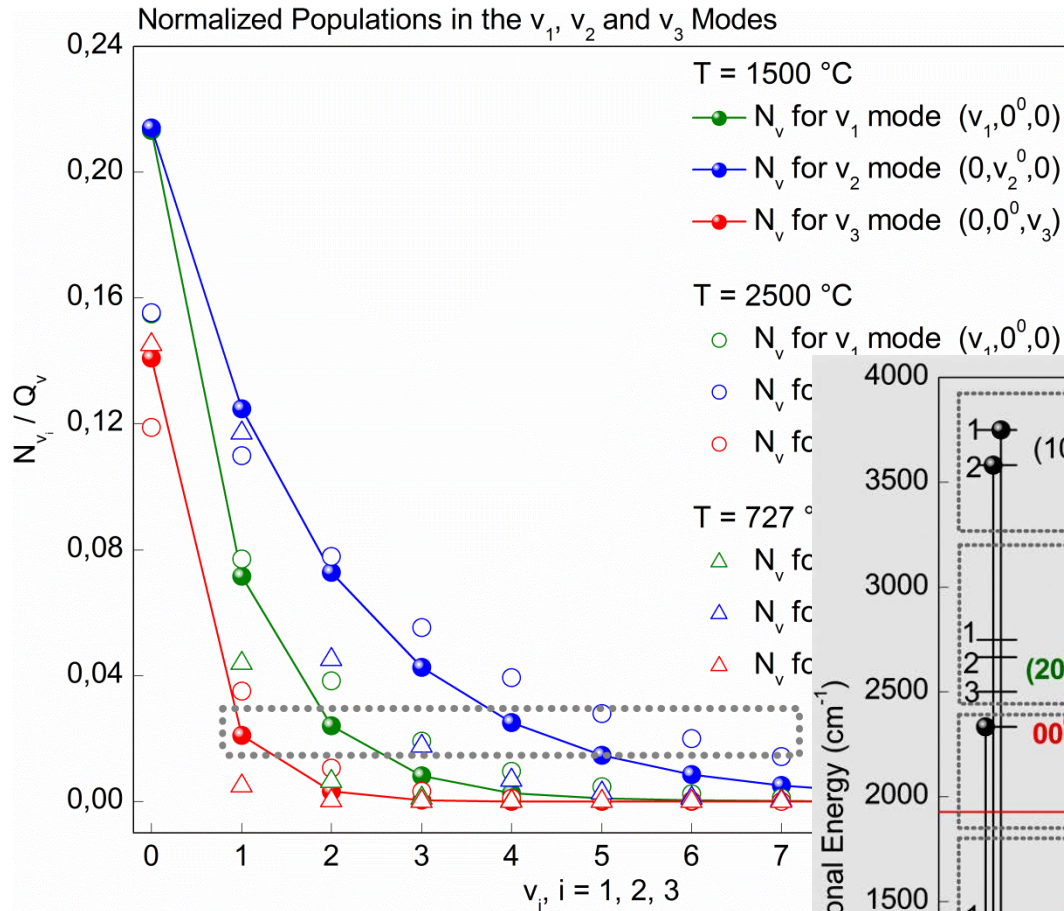
CO₂ transmission spectra: 1500C



CO₂ quasicontinuum at 1500C



CO2 quasicontinuum at 1500C



SO3 project: industry and university

Facts:

- Coal air combustion: SO₂(300ppm) and SO₃(5ppm) (blue smog);
- Large power plants: SCR units (NO_x reduction) with NH₃ injection;
- Global warming: operation at lower loads;
- Lower loads: lower gas temperatures at SCR units;
- By law: not allowed to turn off NH₃ injection system.

Problems:

- Non optimal NH₃ consumption;
- At lower T: H₂SO₄ formation which causes ammonia sulfate and ammonia bisulfate formation;

Consequences:

corrosion in ducts and plugging/damage of SCR elements.

Goal:

to develop an optical method for SO₃ *in situ* measurements.

SO3 project: industry and university

Challenges of the project:

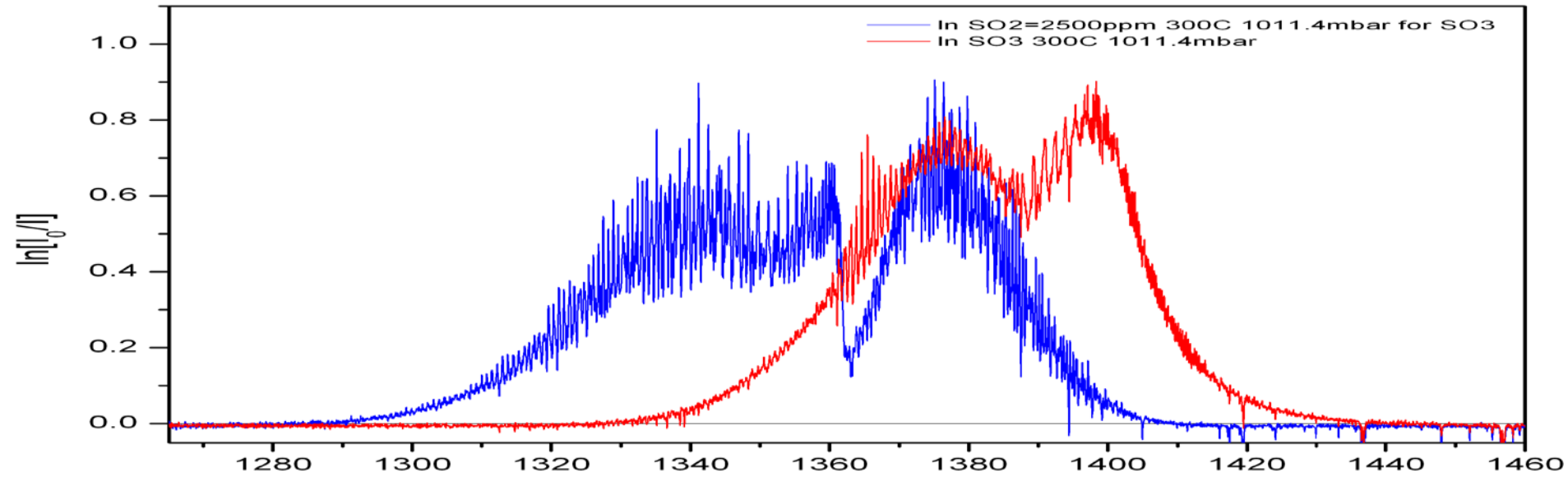
- temperature range 200-500C;
- SO3 high-resolution spectra (SO3 generation);
- SO2, NH3, H2SO4 and H2O high-resolution spectra database;
- water cooled optical probe development;
- powerful IR light source development;
- high sensitivity FTIR with linearized MCT or InSb detector;
- use of modern mathematical tools (e.g. SVD, NNLS).

Two phases of the project:

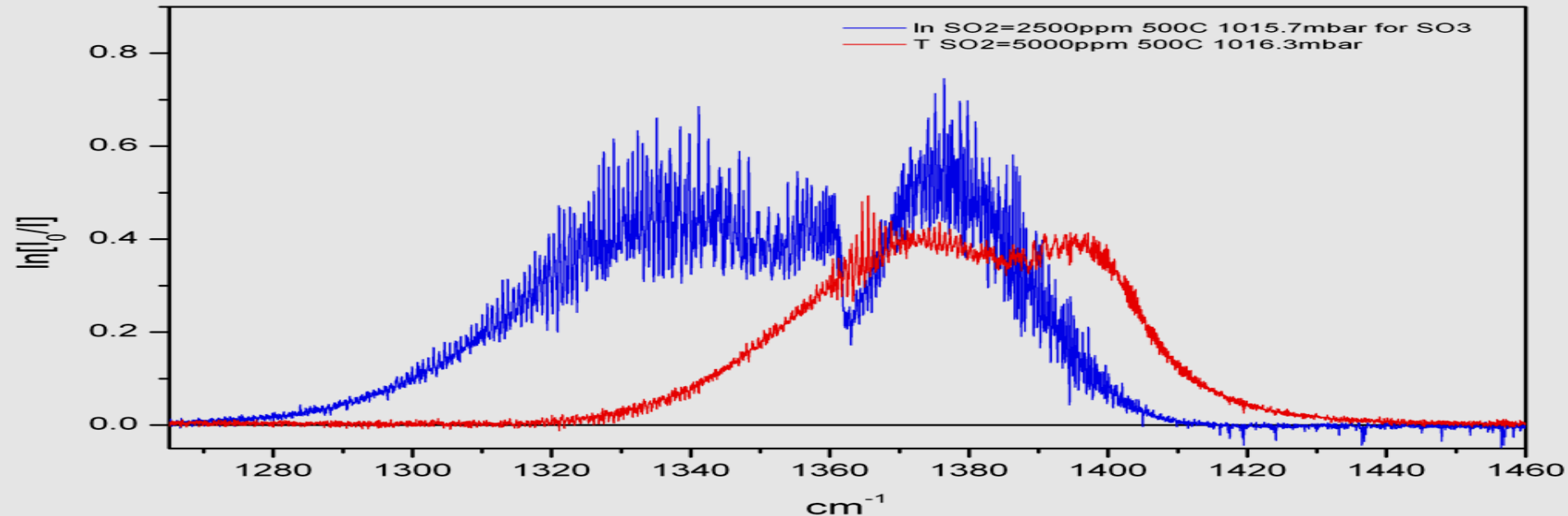
- measurements in the lab and SO2/SO3 line list generation (UCL, UK)
- measurements on an industrial scale (power plant, Dong Energy, DK)

SO3 project: high-resolution (0.115 cm⁻¹) measurements

T=300C

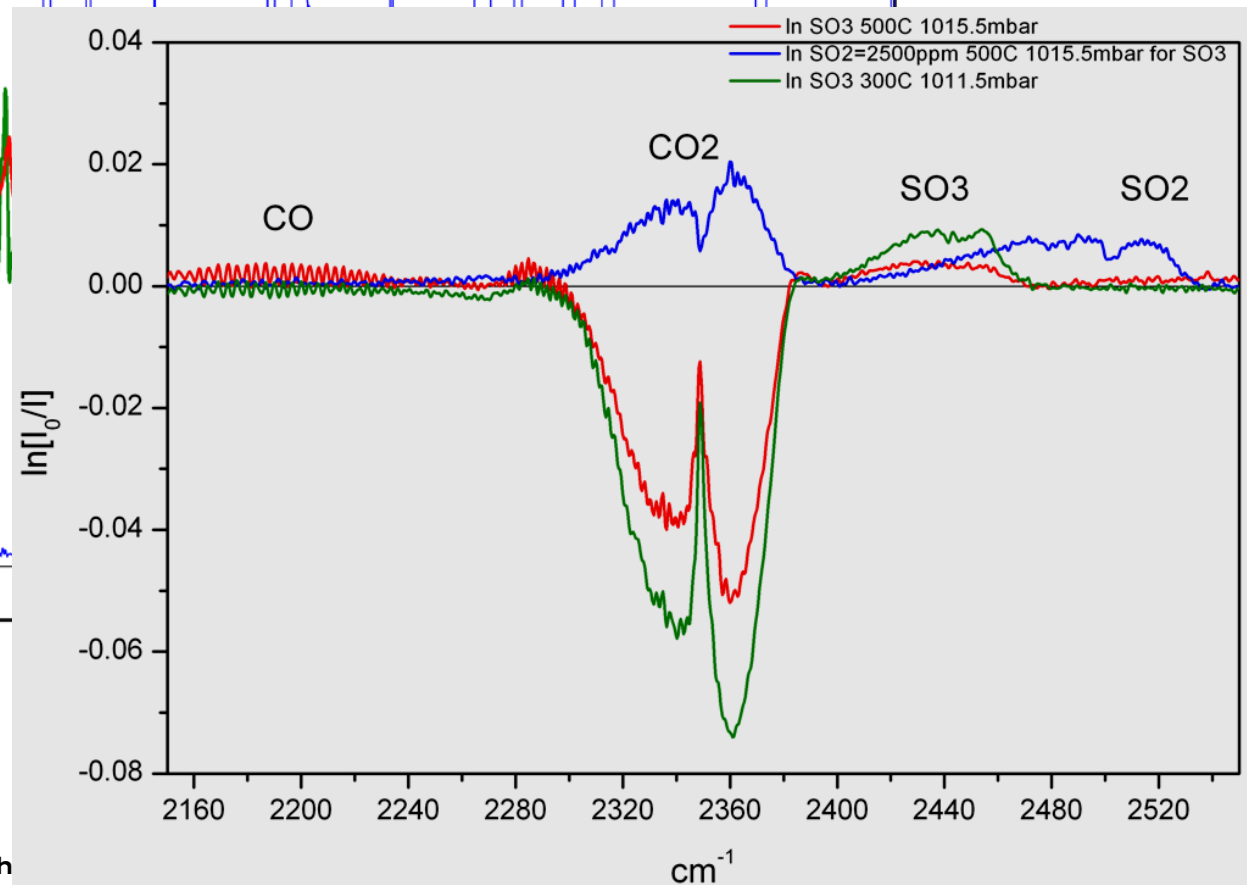
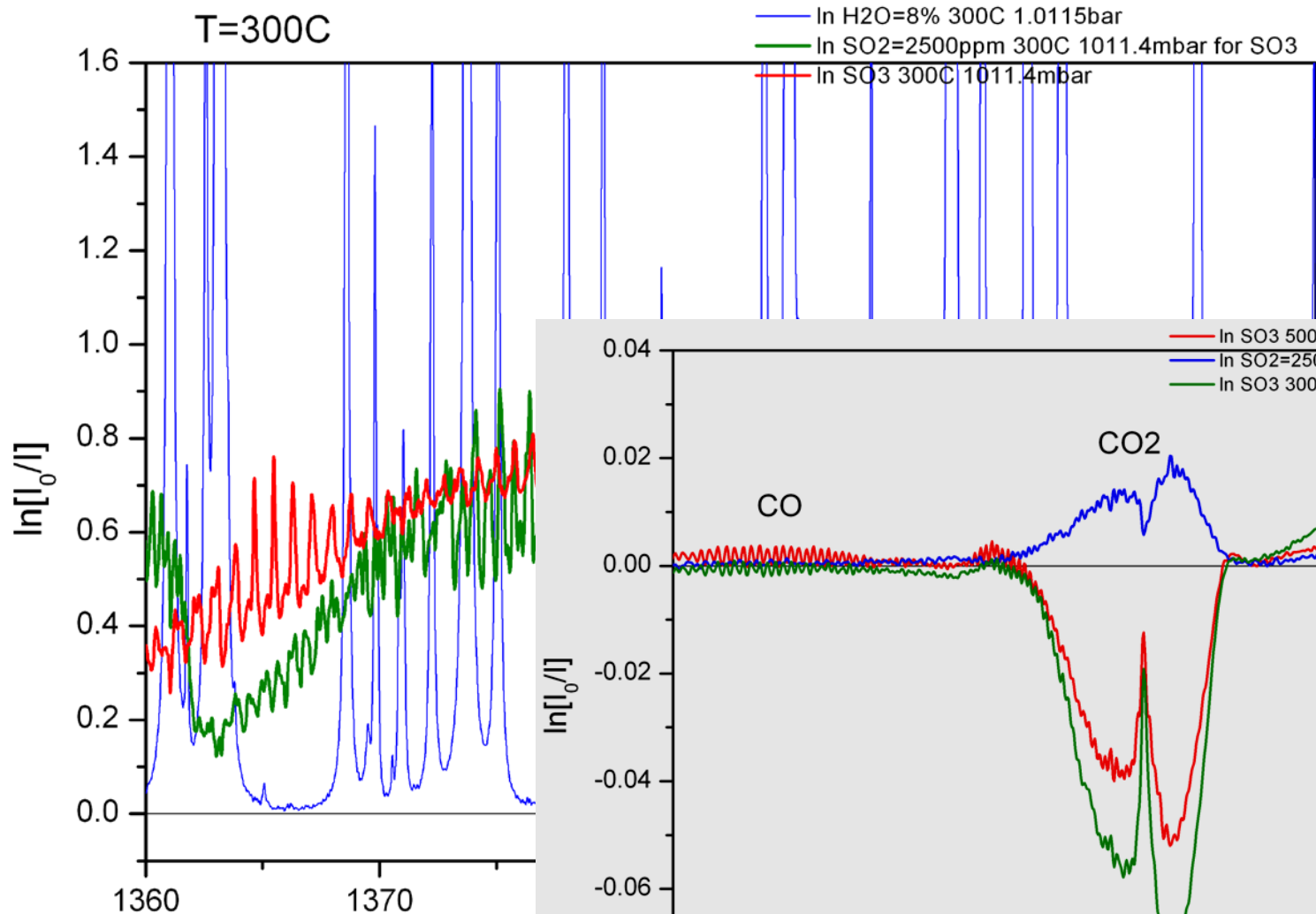


T=500C



SO3 project: interferences

T=300C



Conclusions

High quality optical measurements with various gases (incl. highly corrosive gases) are possible;

A new gas cell is under development (<200 bar, 2000°C)

Measurements can be used for: databases development and validation, studies of chemical reactions, energy exchange, validation of line shape models.

SO3 project is under development: lab work + PhD student employed by UCL;



Acknowledgements

- Energinet.dk: project No. 2010-1-10442
- Dong Energy (Mr. Jan N. Hvidberg)
- UCL (Prof. Jonathan Tennyson)